Isostatic phase transition and instability in stiff granular materials.

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Structural rigidity concepts are used to understand the origin of instabilities in granular aggregates. It is first demonstrated that the contact network of a noncohesive granular aggregate becomes exactly isostatic when $I=k\epsilon/f_l>1$, where k is stiffness, ϵ is the typical interparticle gap and f_L is the typical stress induced by loads. Thus random packings of stiff particles are typically isostatic. Furthermore isostaticity is responsible for the anomalously large susceptibility to perturbation observed in granular aggregates. The load-stress response function of granular piles is critical (power-law distributed) in the isostatic limit, which means that slight overloads will produce internal rearrangements.

Photoelastic visualization experiments [1–3] show clearly defined stress-concentration paths in non-cohesive granular materials under applied load. These often suffer sudden rearrangement on a global scale when the load conditions are slightly changed, evidencing a degree of susceptibility to perturbation not usually present in elastic materials. It is rather possible that this intrinsic instability be responsible for much of the interesting phenomenology of granular materials [3,4]. Recently a number of phenomenological models [2,5–8] have been put forward, which succeed to reproduce several aspects of stress propagation in granular systems, and the issue of instability has been addressed by noting that the loadstress response function may take negative values [6]. It is the purpose of this letter to show that structural rigidity concepts help us understanding the origin of instability in granular materials, linking it to the topological properties of the system's contact network.

Structural rigidity [9] studies the conditions that a network of points connected by rotatable bars (representing central forces) has to fulfill in order to sustain applied loads. A network with too few bars is *flexible*, while if it has the minimum number required to be rigid it is *isostatic*. Networks with bars in excess of minimal rigidity are *overconstrained*, and are in general *self-stressed*. Concepts from structural rigidity were first introduced in the study of granular media by Guyon et al [10], who stressed that granular systems are not entirely equivalent to linear elastic networks since in the former only compressive interparticle forces are possible. We next show that this constraint has far-reaching consequences for the static behavior of stiff granular aggregates.

Consider a d-dimensional frictionless granular pile in equilibrium under the action of external forces \vec{F}_i (gravi-

tational, etc) on its particles. Imagine building an equivalent linear-elastic central-force network (the contact network), in which two sites are connected by a bond if and only if there is a nonzero compression force between the two corresponding particles. Because of linearity, stresses f_{ij} on the bonds of this equivalent system can be decomposed as $f_{ij} = f_{ij}^{self} + f_{ij}^{load}$ where f_{ij}^{self} are self-stresses, and f_{ij}^{load} are load-dependent stresses. These last are linear in the applied load and are do not change if all stiffnesses are rescaled. Self-stresses in turn do not depend on the applied load, but are linear combinations of terms of the form $k_{ij}\epsilon_{ij}$ where k_{ij} are the stiffnesses of the bonds, and ϵ_{ij} their length-mismatches. In a granular pile, length-mismatches are due to interparticle gaps, and therefore will depend on the distribution of radii and on the characteristics of the packing. Furthermore, self-stresses can only arise within overconstrained subgraphs [9,10], i.e. those with more contacts than strictly necessary to be rigid. It is easy to see that a bounded overconstrained subgraph with nonzero self-stresses must have at least one negative (traction) self-stress. It suffices to consider a joint belonging to the envelope of the overconstrained cluster: since bonds can only reach it from one side of the frontier, stresses of both signs are necessary in order for the joint to be equilibrated. Now rescale all stiffnesses according to $k \to \lambda k$. In doing so, self-stresses are rescaled by λ , but load-dependent stresses remain constant. Thus if self-stresses were nonzero, in the limit $\lambda \to \infty$ at least one bond of the network would have negative total stress, which is a contradiction. Therefore stiff granular piles must must either: a) have zero length-mismatches, or b) have no overconstrained graphs at all. Condition a) cannot be satisfied if the particles have random polydispersity, no matter how small, or if the packing is disordered. Therefore there can be no overconstrained subgraphs in polydisperse or disordered packings in the large-stiffness limit. In other words: the contact network of a granular packing becomes isostatic when the stiffness is so large that the typical self-stress, which is of order $k\epsilon$, would be much larger than the typical load-induced stress f_L [11].

The isostaticity condition above is perhaps simpler to understand when cast in the following terms: granular packings will only fail to be isostatic if the applied compressive forces are strong enough to close interparticle gaps establishing redundant contacts.

Thus, real disordered packings will typically be isostatic (interparticle gaps are large) unless its particles are strongly deformed by the load. This explains why the average coordination number of random sphere packings is usually close to 6 (see [10] and references therein). Isostaticity was also reported in numerical simulations of rigid disks [12].

Finally we note that an adimensional "isostaticity parameter" can be defined as $I = k\epsilon/f_L$, and that I >> 1 corresponds to the isostatic limit.

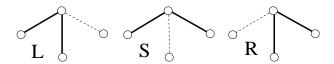


FIG. 1. Appropriately choosing among these three isostatic configurations for each site, only compressive stresses are produced on a triangular packing. First S is chosen with probability 1/2. If S is not chosen then either R or L are, depending on the sign of the horizontal force acting on the site.

We now discuss the consequences of isostaticity for the static behavior of a pile. It is possible to obtain useful insight from recent studies of the related problem of central-force rigidity percolation [16]. Rigid backbones are found to be composed of large overconstrained clusters, isostatically connected to each other by critical bonds (also called red bonds). Cutting one critical bond is enough to produce the collapse of the entire system, because each of these is by definition essential for rigidity. In percolation backbones though, the number of such critical bonds is not extensive, but scales at p_c as $L^{1/\nu}$ where ν is the correlation-length exponent [13]. Thus, if we perturb (cut or stretch) a randomly chosen bond in a percolation backbone, most of the times the effect will be only be local since no critical bond will be hit. The new element in stiff granular contact-networks is the fact that all contacts are isostatic, or critic, i.e. there is extended isostaticity. Thus we may expect stiff granular systems to have a large susceptibility to perturbation since cutting (stretching) a bond will often produce a large part of the system to collapse (move).

Let us now quantify these ideas. We perturb the system by introducing an infinitesimal change δl in the length of a randomly chosen bond, and record the induced displacement $\delta \vec{x}_i$ suffered by particle centers in equilibrium. The system's susceptibility to perturbation is then defined as $D = \sum_{i=1}^N |\delta \vec{x}_i/\delta l|^2$. We propose to measure $D(O_v)$ as a function of the density O_v of overconstraints (excess contacts) randomly located on the network. Isostatic piles have $O_v = 0$.

A simple one-dimensional model for the propagation of perturbations can be analytically solved [17] for arbitrary values of the density O_v of overconstraints. For any non-zero O_v , D as defined above takes a finite value, but diverges as $O_v^{-1/2}$ for $O_v \to 0$. Therefore there is a phase transition at the isostatic point $O_v = 0$.

We now analyze a two dimensional system numerically. In the spirit of previously studied models [14], we consider a triangular packing of H layers height, with one of its principal axis parallel to gravity, and made of disks with small random polydispersity δR and weight W. Since δR is small, disk centers are approximately located on the sites of a regular triangular lattice. If the stiffness k is large enough $(I = k\delta R/WH >> 1)$, the contact network will be isostatic. We enforce isostaticity in our model by letting each site be supported from below by only two out of its three neighbors. This gives three possible local configurations which are depicted in Fig.1. By appropriately choosing among these [17], random isostatic networks with only compressive stresses are generated. In order to study the effect of a finite density O_v of overconstraints (which would appear if the stiffness is lowered), we furthermore let all three bonds be present with probability O_v at each site.

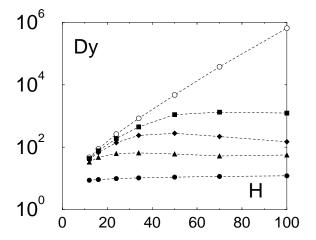
After building a disordered network in this way, a randomly chosen bond in the lowest layer is stretched, and the induced displacement field is measured. After averaging over disorder, the stress distribution [17] is found to decay exponentially for large stresses, in accordance with previous work [2,15].

The results for the susceptibility $D_y(H, O_v) = \sum_{i=1}^{N} \delta y_i^2$ are shown in Fig. 2a. Here δy_i is the vertical displacement of site i due to a unitary bond-stretching, as measured on packings of $N = H \times H$ particles. For $O_v > 0$, D_y goes to a finite limit for large sizes H, but diverges with system size if $O_v = 0$. Measurements on isostatic packings of up to H = 2000 layers [17] show that $\log D_y \propto H$, i.e. the divergence of D_y is exponential with size when $O_v = 0$. Thus there is a surprising phase transition at $O_v = 0$, where anomalously large susceptibility sets in.

In order to understand how displacements propagate upwards, we measure the probability distribution $P_h(\delta y)$ to have a vertical displacement δy , h layers above the perturbation. Numerical results for isostatic systems with H=2000 are shown in Fig. 2b. For large h, $P_h(\delta y)$ decays as a power-law with an h-dependent cutoff: $P_h(\delta y) \sim h^{-\rho} |\delta y|^{-\theta}$, $\delta y < \delta_M(h)$. As seen in Fig. 2b, $\delta_M(h)$ grows exponentially with height h. This produces the observed exponential divergence of D_y . Similar measurements were done on systems with a finite density of overconstraints O_v , in which case the distribution of displacements presents a height-independent bound [17].

The puzzling appearance of exponentially large displacements on isostatic piles can be explained as due to the existence of "lever configurations" or "pantographs", which amplify displacements. Fig. 3 shows an example of a pantograph with amplification factor 2. Given that this and similar mechanisms appear with a finite density per layer, it is clear that the second moment of $P_h(\delta y)$ will grow exponentially with system height. Fur-

thermore, it is easy to understand why this amplification effect only exists in the *isostatic limit*: Pantographs as the one in Fig. 3 are no longer effective if blocked by overconstraints, for example if an additional bond is added between site A and the site below it. In this case, a stretching of bond B would induce stresses in the whole pantograph, and only a small displacement of site A.



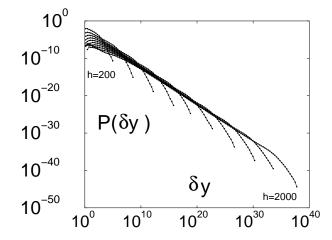


FIG. 2. a) Total susceptibility D_y versus system height H in layers, as numerically measured on two-dimensional triangular packings. The fraction of overconstraints (fraction of sites supported by three lower neighbors) is: 0.00 (open circles), 0.01 (squares), 0.02 (diamonds), 0.05 (triangles) and 1.00 (full circles). b) The probability $P_H(\delta y)$ to have an induced vertical displacement δy , H layers above the perturbation, as obtained in a numerically exact fashion for the isostatic ($O_v = 0$) triangular piles described in the text. Results are shown for $H = 200, 400, 600, \ldots, 2000$. Only positive values of δy have been plotted here.

In order to formalize the relationship between these findings and the observed unstable behavior [1,2] of granular materials, we now demonstrate the equivalence between induced displacements and the load-stress response function [6] of the stretched bond. The network's total energy can be written as $E = \sum_{i=1}^N W_i y_i + 1/2 \sum_b k_b (l_b - l_b^0)^2$ where the first term is the potential energy and the second one is a sum over all bonds and accounts for the elastic energy. l_b are bond lengths in equilibrium and l_b^0 their repose lengths. Upon infinitesimally stretching bond b', equilibrium requires that $\sum_i W_i \frac{\partial y_i}{\partial l_{b'}} + \sum_{ov} k_{ov} (l_{ov} - l_{ov}^0) \frac{\partial l_{ov}}{\partial l_{b'}} = 0$, where the second sum goes over bonds ov that belong to the same overconstrained graph as b' does. This is so since bonds not overconstrained with respect to b' do not change their lengths as a result of stretching b'. Since stress f_b on bond b is $f_b = k_b (l_b^0 - l_b)$ this may be rewritten as

$$\sum_{ov} f_{ov} \frac{\partial l_{ov}}{\partial l_{b'}} = \sum_{i} W_{i} \frac{\partial y_{i}}{\partial l_{b'}} \tag{1}$$

If b' does not belong to an overconstrained graph, the left hand sum only contains bond b' itself, therefore $f_b = \sum_i W_i \frac{\partial y_i}{\partial l_b}$ showing that, in the isostatic case (no overconstrained graphs at all), the induced displacement $\delta y_i^{(b)} = \frac{\partial y_i}{\partial l_b}$ is equal to the response function of stress f_b with respect to an overload on site i.

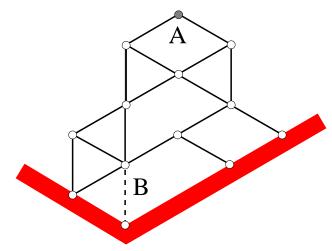


FIG. 3. The observed exponential growth of induced displacements is due to the existence of random "pantographs" as the one shown in this figure. Upon stretching bond B by an amount δ , site A moves vertically by an amount 2δ . Conversely a unitary weight at A produces a stress of magnitude 2 on bond B. This is a consequence of the general equivalence between induced displacements and the load-stress response function.

Taking averages with respect to disorder we obtain $\langle f_b \rangle = \sum_i W_i \langle \delta y_i^{(b)} \rangle$ and since average stresses grow as H we must have $\langle \delta y_i^{(b)} \rangle \sim H^{-1}$. We thus see that there must be delicate cancellations in $P(\delta y)$, since its second moment diverges as $\exp\{H\}$ while its first moment goes to zero with H. This shows that δy (and therefore the response function) takes exponentially large values of both signs, $(P(\delta y))$ is approximately symmetric).

Thus a positive overload at site i would often produce a (very large) negative stress on bond b, implying the need for rearrangement since negative stresses are not allowed.

The existence of negative values for the response function was first discussed in relation with instability, in the context of a phenomenological vectorial model for stress propagation [6]. The results of the present work demonstrate that the response function takes exponentially large negative values, and the system is unstable, because of the isostatic character of the contact network.

To conclude, we have shown that granular packings are exactly isostatic when $I = k\epsilon/f_L$ is much larger than one, which holds for typical disordered packings, and also for stiff enough regular packings with random polydispersity.

For isostatic packings, the distribution of displacements induced by a perturbation is power-law with an exponentially large cutoff. A susceptibility to perturbation can be defined, which diverges upon increasing I. Thus, an isostatic phase transition takes place in the limit of large I.

Induced displacements were furthermore shown to be equivalent to the load-stress response function of the perturbed bond. Our results for induced displacements thus mean that response functions take exponentially large values, as well positive as negative, in the isostatic limit. This explains why stiff granular piles are unstable. Any non-zero density of overconstraints destroys criticality and therefore instabilities will not be present when the isostaticity parameter I is small. I can be reduced by reducing the stiffness, the interparticle gaps, or by increasing the load.

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